# Smoke Chemistry

Michael F. Borgerding, Ph.D.
R. J. Reynolds Tobacco Company

## Reduced Risk Smoke Chemistry

- **Less Ought To Be Better**
  - Measurement of General Smoke Yields (e.g., FTC "Tar")
- **Simpler Ought To Be Better**
  - Study of Smoke Composition

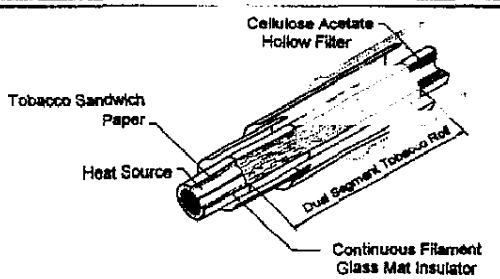
## As Innovative Technologies Introduced in Cigarette Design:

- Amount of Tobacco Burned to Form Mainstream Smoke has Decreased (Reduced "Tar" Yields)
- Composition of "Tar" Remained Generally Constant

## Principal Smoke Formation Mechanisms

- When Burning Tobacco
  - Combustion
  - Pyrolysis
  - Pyrosynthesis
  - Vaporization / Condensation
- When Primarily Heating Tobacco (Eclipse)
  - Combustion
  - Pyrolysis
  - Pyrosynthesis
  - **Vaporization / Condensation**

## An Example for Assessing Harm Reduction - The *Eclipse* Cigarette




## Effect of Cigarette Design Technologies on Smoke Composition

| The Past 40 Years | Eclipse |
|---|---|
| Composition of "Tar" has Remained Generally Constant | Significantly Different "Tar" Composition |



Source: https://www.industrydocuments.ucsf.edu/docs/hgdk0001

## Chemical Analysis Strategy

- Standard Smoke Measures (FTC Method)
- Gross Measures
- Aggregate Chemical Measures
- Specific Compound Determinations

## (1) Standard Smoke Measures

- FTC Method
  - "tar"
  - nicotine
  - puff count
  - carbon monoxide

## Machine Based Testing

- Cigarette smoke is produced and compared under constant machine-generated conditions
- FTC Puffing Regimen
  - 35 cc Puff Volume
  - 2 s Puff Duration
  - 1 Puff Every 60 s
  - Standard Cigarette Butt Length Spec.

## What is "Tar"?

## Choice of Cigarettes

- Equivalent "tar" comparison
- Comparison of multiple "tar" categories

## Cigarettes Evaluated

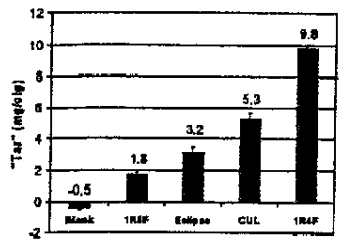
- Eclipse
- CUL Brand
- Kentucky 1R4F
- Kentucky 1R5F
- Blank

- Test Cigarette
- Commercial "Ultra Light"
- Reference "Light"
- Reference "Ultra Light"
- Sham Smoking

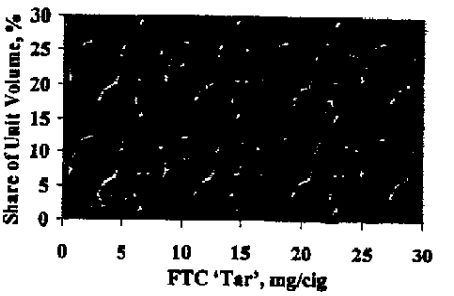


Source: https://www.industrydocuments.ucsf.edu/docs/hgdk0001

## FTC "Tar" Yields




## Share of Volume by 'Tar' Yield

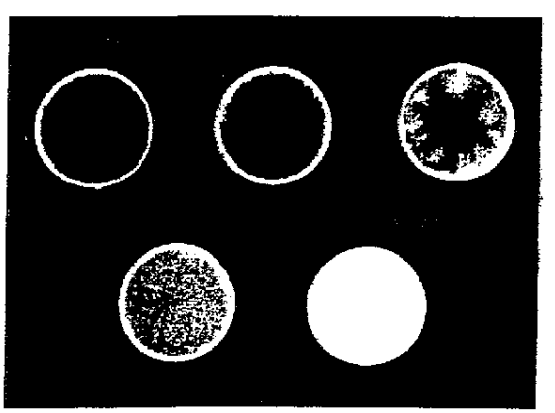



## (2) Gross Measures

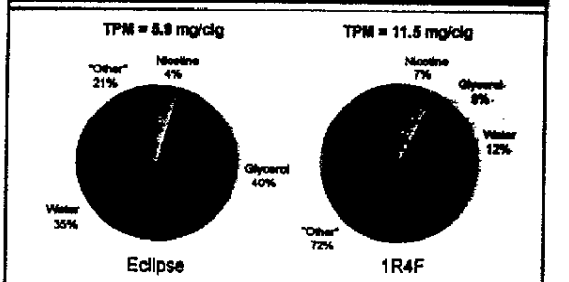
Measurements based on a chemical or physical property of smoke total particulate matter

## Examples of Gross Measures

- Elemental Composition (C,H&N)
- UV Absorption
  - Spectrophotometric "tar"
- Thermogravimetric Analysis
  - volatility
  - stability
- Materials Balance Assessment
- Visual Comparison



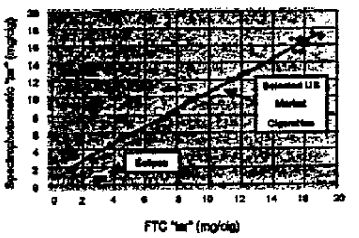
## Materials Balance Comparison




PM3001242804

Source: https://www.industrydocuments.ucsf.edu/docs/hgdk0001

## Comparison of Spectrophotometric and FTC "Tar" Determinations



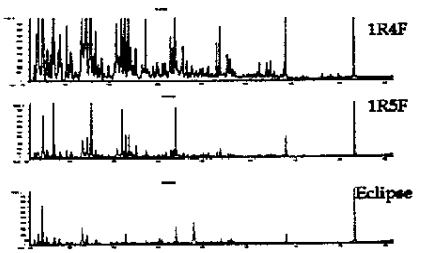

## (3) Aggregate Measures

- Address an open ended question
- Collective response from many compounds, rather than single chemical
- Comparative measure

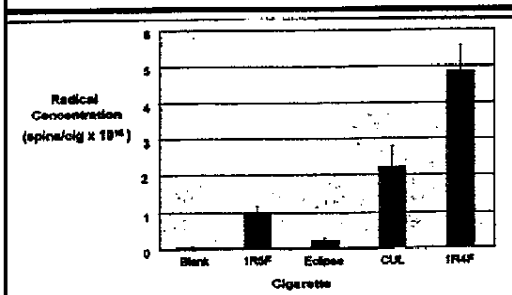
## Aggregate Chemical Measures

- Chromatographic Profiling
  - Vapor Phase
    - Number of Peaks
    - Total Peak Response
  - Particulate Phase
    - Number of Peaks
    - Total Peak Response
- Vapor Phase Free Radicals

## Chromatographic Profiling - Vapor Phase Comparison




## Vapor Phase Radical Response




## (4) Specific Compound Determinations

- "Target Compound" Determinations
  - Closed ended question
  - Determine amounts of specific chemicals
  - Absolute measures

PM3001242805

Source: https://www.industrydocuments.ucsf.edu/docs/hgdk0001

## "Target Compounds" Studied

- ~ 30 Specific Chemicals or "Target Compounds" Studied
  - Represent Broad Range of Chemical Classes
- Compounds Studied Based on Literature
  - US Surgeon General's Report
  - IARC Monograph
  - Consumer Product Safety Commission

## "Target Compounds" Studied

- Carbonyls
  - Formaldehyde
  - Acetaldehyde
  - Acetone
  - Acrolein
- Hydroxybenzenes
  - Phenol
  - Cresols
  - Catechol
  - Hydroquinone

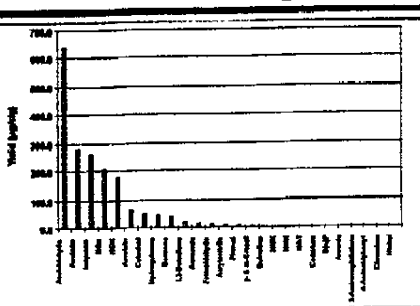
## "Target Compounds" Studied

- Aromatic Amines
  - 2-aminonaphthalene
  - 4-aminobiphenyl
- TSNAs
  - NNN
  - NAT
  - NNK
- Inorganic
  - Aluminum
  - Arsenic
  - Cadmium
  - Chromium
  - Nickel
  - Silicon

## "Target Compounds" Studied

- PAH
  - Benzo(a)pyrene
- Aza-arenes
  - Quinoline
- Misc. Organic
  - Benzene
  - Acrylonitrile
- Miscellaneous
  - Ammonia
  - Nitrogen Oxides
  - HCN
- Unsat. Hydrocarbons
  - Isoprene
  - 1,3-Butadiene

## Relative Target Compound Yields for a Low "Tar" Cigarette



## Eclipse Target Compound Reductions

| | Percent Reduction when Compared to: | | |
|---|---|---|---|
| | 1R5F | CUL | 1R4F |
| B(a)P | -63 | -86 | -90 |
| Carbonyls | -36 | -72 | -86 |
| HCN | -57 | -90 | -95 |
| Phenolics | -88 | -97 | -98 |
| Nitrosamines | -50 | -81 | -82 |
| $NO_x$ | -48 | -72 | -84 |



Source: https://www.industrydocuments.ucsf.edu/docs/hgdk0001

## Alternative Puffing Regimen Data

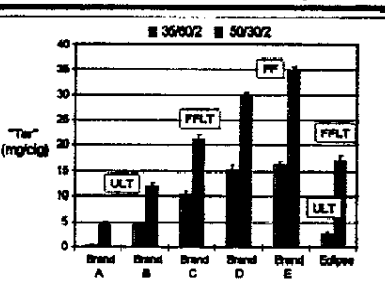
## Rationale for Alternative Puffing Regimen Studies

- Standard Machine Smoking Methods Have Been Criticized in Recent Years
  - NCI Expert Committee (1994)
  - FTC Proposed Changes to Method
- Numerous Alternative Puffing Regimens Have Been Recommended
  - Thought by Some Researchers to Better Represent "Human Smoking Conditions"

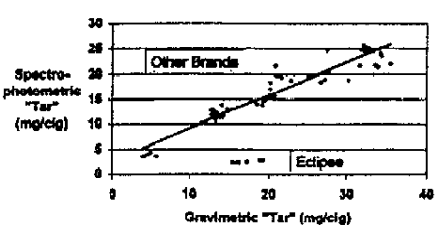
## Other Smoking Conditions Considered Recently

| Puff Volume (cc) | Puff Frequency (s) | Puff Duration (s) | Filter Ventilation Condition |
|---|---|---|---|
| 35 | 60 | 2 | "open" |
| 45 | 34 | 2 | 50% "blocked" |
| 60 | 26 | 2 | 100% "blocked" |

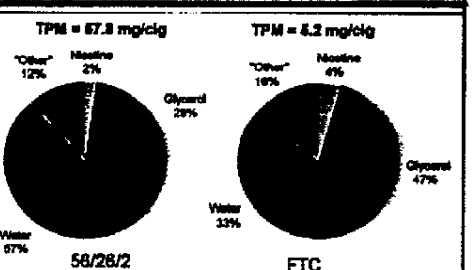
## Relative "Tar" Ranking - Eclipse and Other U.S. Cigarettes




## Spectrophotometric "Tar" - 50/30/2 Puffing Regimen




## Materials Balance Comparison - Eclipse




PM3001242807

Source: https://www.industrydocuments.ucsf.edu/docs/hgdk0001

## General Finding

- Simpler Eclipse mainstream smoke chemistry found with FTC smoking regimen was also observed for the other smoking conditions studied

## Summary

## Chemical Analysis Strategy

Smoke Yields

1 Standard Smoke Measures ("Tar," Nicotine, Carbon Monoxide)

Smoke Composition

2 Gross Measures

3 Aggregate Chemical Measures

4 Specific Compound Determinations

## Reduced Risk Smoke Chemistry

- **Less Ought To Be Better** → Measurement of General Smoke Yields (e.g., FTC "Tar")
- **Simpler Ought To Be Better** → Study of Smoke Composition

## Effective Strategy for Assessing Risk Reduction in Cigarettes

Reduction of Chemical Substances

✓ Smoke Chemistry Studies

Less Toxicity

- In Vitro Toxicity Studies
- Animal Toxicity Studies

Reduced Effects in Smokers

- Smoking Behavior/Exposure Assessment
- Clinical Studies using Surrogate Markers

## Smoke Chemistry

Michael F. Borgerding, Ph.D.
R. J. Reynolds Tobacco Company



Source: https://www.industrydocuments.ucsf.edu/docs/hgdk0001